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University Research Core Facility Boilerplate
Descriptions

Office of Research and Partnerships

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Macromolecular Crystallography

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Macromolecular Crystallography

https://www.cancerresearch.purdue.edu/for_researchers/macromolecular_cryst.html

Hockmeyer Hall of Structural Biology, Rooms 284 and 289

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The Hockmeyer Hall Macromolecular Crystallization and X-ray Diffraction Laboratories are used by Purdue researchers to determine the molecular structures of proteins, viruses, and nucleic acids by X-ray crystallography. Anticipating hands-on use by students, staff, and faculty, the essential service of this resource is to provide facilities for macromolecular crystallography. The facilities include instruments required for the measurement of single crystal diffraction patterns and for the semi-automated crystallization of macromolecules. To achieve this service, an experienced technical staff maintains the facilities, and a resource director provides scientific guidance in the development of materials and the use of the instruments.

Equipment in the Crystallization Facility includes:

- A Genomics Solutions Cartesian 'Honeybee' 963 liquid handler configured to pipette 96+1 or 96+3 SMB style plates allows rapid and complete screening of crystallization space. Fifteen Qiagen crystallization reagent screens are available for screening. Thus the initial evaluation of a new protein or complex can be accomplished in a few hours, testing the 15 reagent sets against three different protein or protein:ligand concentrations for a total of over 4000 experimental conditions.
- A Rigaku/Robodesign Desktop Minstrel temperature-controlled crystallization "hotel" is available to monitor and document crystallization trials. This instrument has the hardware and software to monitor and record crystal growth and track experimental variables and metadata. These records are available through a dynamic web page that allows visualization and scoring of the trials on workstations across campus.
- A Rigaku/Robodesign Alchemist liquid handling robot is integrated into the Rigaku CrystalTrak software automating the creation of ad-hoc deep well blocks, which are often used in experiments that follow a screening lead.
- A 4DX-ray Systems micro-spectrophotometer allows optical monitoring of binding and catalysis experiments in crystals or other small volume samples.
- Three walk-in incubator rooms with storage cabinets designed to provide low-vibration, temperature-controlled environments are available for incubation of crystallization apparatus at fixed temperatures of 20, 12, and 4 °C (± 0.5 °C). Three free-standing incubators are available for experiments at other temperatures. All rooms and incubators are monitored by a digital scanning thermometer with a software system that logs and displays temperature data and provides warning messages by e-mail. Good to excellent light microscopes are present in each of the 20, 12, and 4 degree rooms; those in the 20° room are equipped with digital camera or video systems.

Equipment in the Diffraction Laboratory includes:

- One R-axis-IV++ imaging plate diffractometer is served by a Rigaku RU-H2R X-ray generator equipped with a Cu rotating anode, a 100 μ m focal assembly,

and MSC Hires² multilayer optics. This system is optimized for the separation of reflections from crystals with a long unit cell axis.

- A second R-axis-IV++ imaging plate diffractometer is served by a Rigaku RU-200 X-ray generator equipped with a Cu rotating anode, a 300 μm focal assembly, and MSC Blue multilayer optics.
- Both diffractometers are equipped with dry N₂ gas cryogenic crystal cooling systems, and both have inverted crystal rotation assemblies to simplify mounting and dismounting of cryogenically preserved crystals.
- A wide variety of shared and private computational resources are available to support the analysis, management, and preservation of diffraction data. All computational resources and the diffraction instruments are accessible through the campus network.

The Macromolecular Crystallography Shared Resource operates within the framework of a University-approved recharge center in compliance with relevant University and external guidelines. The recharge mechanism provides fiscal management of a facility such as this one that depends on varied sources of income. User fees for the diffraction equipment have been established and are reviewed as needed to reconcile expenses, all sources of income, and use. Walk-in incubators were provided and are maintained through institutional support from Purdue University.

Reserved access to the X-ray diffraction instruments is scheduled through a continuous, web-based calendar tool. Each funded investigator is allotted a specific number of reservation tokens per instrument, which are used to reserve individual or consecutive instrument days, one day per token. Four reservation tokens are currently allocated per investigator for each instrument per month. Tokens can be re-used once the reserved date is past, and mechanisms are available to further extend quotas if the samples or experiments require a longer block of consecutive days. If an instrument is not reserved, it is available for walk-on use. Given the current excess capacity and usage patterns, the reservation quota does not limit experiments.

Use of the crystallization robotics is currently walk-on with supervision and without charge in order to encourage use and familiarize the faculty with its capabilities. Substantial increases in usage and attendant costs for maintenance and personnel may require the initiation of charges and a reservation system in a manner similar to those for the diffraction equipment.

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